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Pattern-oriented Agent-based Monte Carlo simulation of Cellular Redox Environment

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Introduction

Research suggests that cellular redox environment could affect the phenotype and function of cells through a complex reaction network. In cells, redox status is mainly regulated by several redox couples, such as Glutathione/glutathione disulfide (GSH/GSSG), Cysteine/ Cystine (CYS/CYSS) and mitochondrial redox couples. Evidence suggests that both intracellular and extracellular redox can affect overall cell redox state. How redox is communicated between extracellular and intracellular environments is still a matter of debate. In general, previuous experiments lack insight into the dynamics, complex network of reactions and transportation through cell membrane of redox. Therefore, the experimental results reveal but a snapshot, or average of true dynamics. In our project, an agent-based Monte Carlo modeling is offered to study the dynamic relationship between extracellular and intracellular redox and complex networks of redox reactions[1](see **Fig. 1**), with the spatial distribution of enzymes and reactants in 3D.

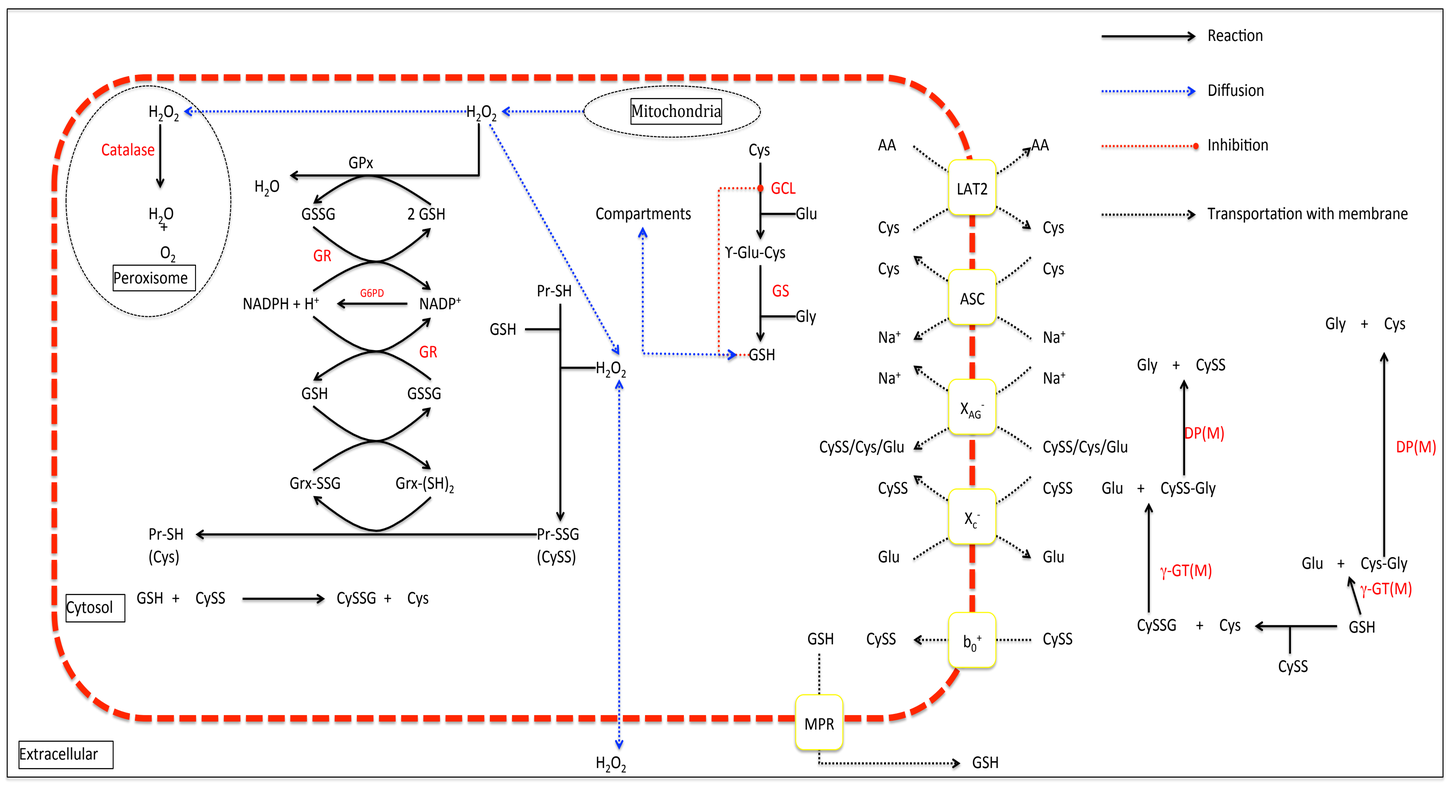

Fig. 1 Redox reaction and transportation networks in our model

Method

The simulation will be done with one spherical cell, which doesn't have subcellular compartments, and bigger spherical extracellular environment.

Our model follows the basic idea about how to simulating reactions with monte carol agent-based modeling[2]. What is more, results of existing experiments will be used to validate the modeling according to ideas in pattern-oriented agent-based modeling[3].

At last, the model will be implemented with an application called "FLAMEGPU", which can be run in NVIDIA graphic card with GPUs based on Compute Unified Device Architecture (CUDA) technology developed by NVIDIA. The modeling and simulation process of "FLAMEGPU" is shown in **Fig. 2.**

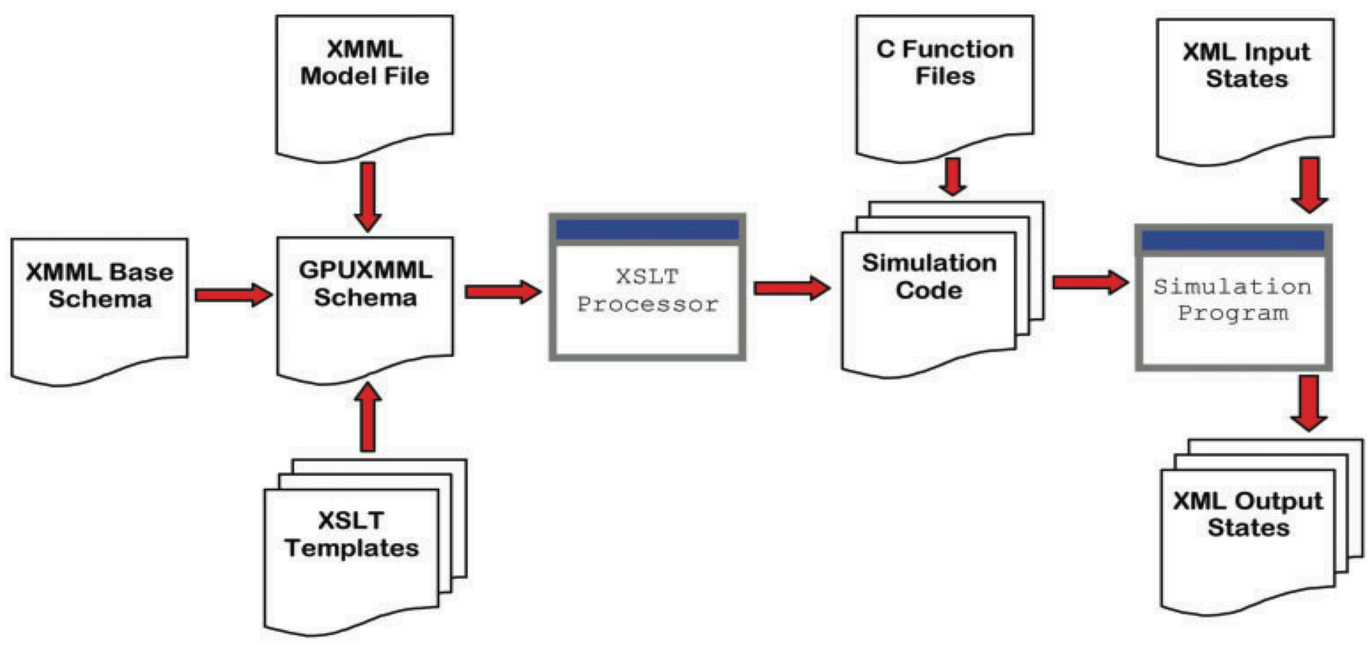

Fig. 2 FLAMEGPU modeling and simulation process[5]

Future work

The model is still in the implementing process. However, in the future, there are still a lot of work to do, such as optimizing the code and model(**Fig. 1**), validating the rules in model with previous experiment and existing mathematical modeling, and interpreting the simulation results with physiological view. In our expectation, our model will be similar the one in [4] if the model will be visualized(see **Fig. 3**).

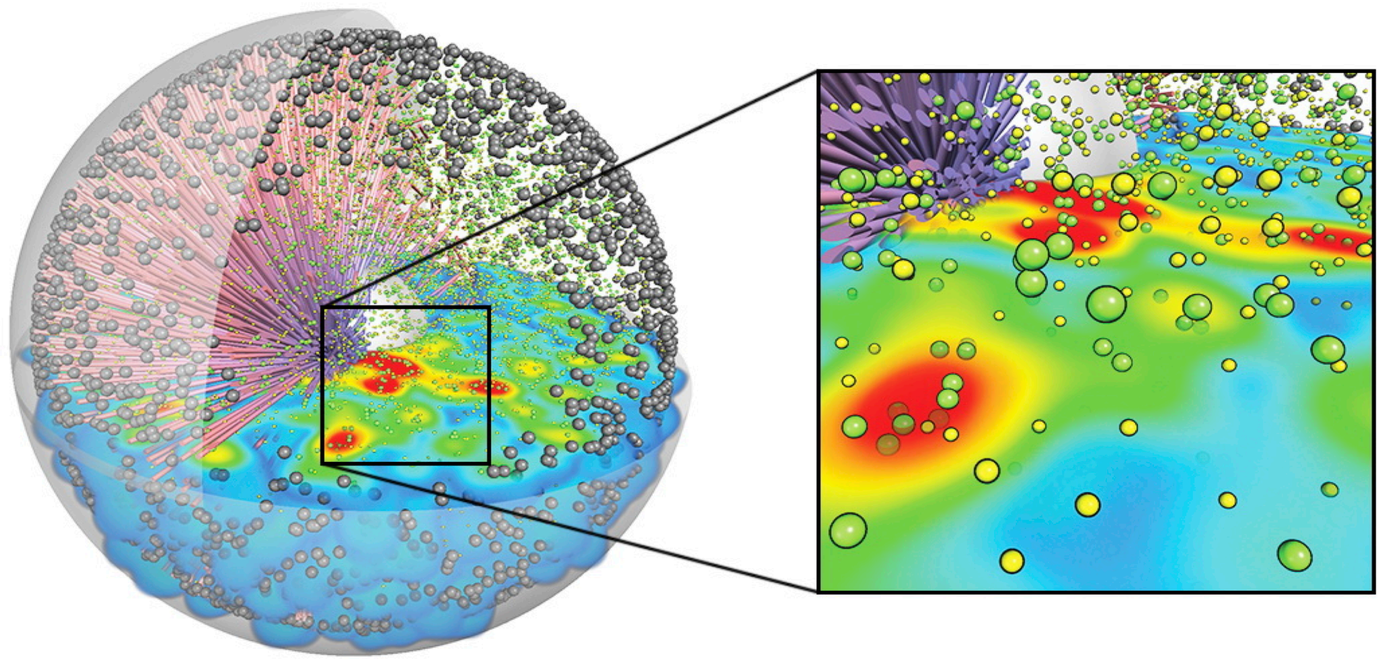

Fig. 3 Visualization of a virtual cell showing the results of a MAPK simulation[4]

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